
Preface

During the first 25-year existence (1990–2015) of the international journal *Structural Chemistry*, it has published hundreds of articles in crystallography. From the start, there has been a characteristic direction in this periodical to bring out reports related to generalized crystallography, quasicrystals, icosahedral packing, other packing considerations, extended structures, data treatment and data mining, and what we would call “living history.”

Several of the contributions came from the schools of such trend-setting crystallographers as J. Desmond Bernal and Aleksandr I. Kitaigorodskii. Internationally renowned scientists have figured as authors, among them, Tom L. Blundell, Johann Jacob Burckhardt, John L. Finney, Jenny P. Glusker, Nobel laureate Herbert A. Hauptman, the 2014 Ewald Prize winner A. Janner, Aminoff Prize winner Isabella Karle, Nobel laureate Jerome Karle, the late doyen of Chinese crystallography K. H. Kuo, Buckley Prize winner Alan L. Mackay, Ewald Prize winner David Sayre, Vladimir Shevchenko, and King Faisal Prize winner J. Fraser Stoddart.

A few frontier topics dominate the selected material in this volume. Pioneers of the direct methods describe the phase problem and how it was solved, including the mathematical approach and the utilization of experience with gas-phase electron diffraction. The reviews by Herbert Hauptman, Jerome and Isabella Karle, and David Sayre reach to the present day in assessing the possibilities of X-ray crystallography.

Another focus topic is the investigation of systems that are outside the so-called classical system of crystals. They include quasicrystals, imperfect and very small crystals, supramolecular species, crystal structures without lattice, clusters, and nanomaterials, among others. The application of synchrotron and cryoprotection techniques, the free-electron laser flash technique, and others is among the techniques of investigation in addition to X-ray crystallography.

The relationship between structural and materials properties is examined and uncovered. The broader topics include polymers, clusters, polydisperse chain assemblies, and giant icosahedral fullerenes. There are some key contributions related to the structural investigation of biological macromolecules. There are packing considerations and work toward one of the ultimate goals of crystallography as a science of structures: to predict crystal structures from the chemical composition of new substances.

A modern tool in structure analysis is data mining and data management. *Structural Chemistry* has paid attention to and attracted authors utilizing the possibilities of data banks, in particular the Cambridge Data Files and the inorganic crystal structure database (ICSD in Karlsruhe). Selected articles in this compilation demonstrate the potentials of the utilization of data banks.

We have arranged the 33 articles selected for inclusion in four parts. However, the classification is blurred as authors do not write articles to correspond to clear-cut classifications. Thus, the distribution of the contributions in this compilation is approximate, and there are overlaps.

The selection process which led us to the 33 articles reproduced here happened in three cycles during which we consulted with others as we were narrowing our choice in a gradual manner.

Only as an aside we note that the authors of the articles come from at least 14 countries (USA, UK, Russia, Hungary, India, Italy, Switzerland, Canada, China, France, Germany, Israel, Mexico, and the Netherlands). That the 33 articles originated from at least 14 countries reflects the international character of the collection although we paid no attention to this aspect in the process of compilation.

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